

# Two-Roton Bound State in the Fractional Quantum Hall Effect

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The true nature of the lowest-energy, long-wavelength neutral excitation of the fractional quantum Hall effect has been a long outstanding problem. In this Letter, we establish that it is a two-roton bound state.

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The neutral excitations of the fractional quantum Hall effect [1] (FQHE) have attracted considerable interest in the last fifteen years since the initial work of Girvin, MacDonald, and Platzman (GMP) [2] in which they used a single mode approximation (SMA) to study the excitations at Landau level filling  $\nu = 1/3$ . The long-wavelength limit, the topic of the present Letter, is of particular interest because of its relevance to Raman scattering experiments [3–6]. In their original work, GMP raised the question of whether the lowest energy excitation at long wavelengths was described correctly by the SMA or was instead a two-roton excitation. Despite some further work [7], this question has remained unresolved until now, both because of the lack of a quantitative theory of the two-roton excitation and because the system sizes on which exact-diagonalization studies can be performed are too small to shed meaningful light on long wavelength excitations. We wish to show that recent developments in the composite fermion theory have made it possible to provide a definitive answer to this question.

A composite fermion (CF) is the bound state of an electron and an even number of magnetic flux quanta (a flux quantum is defined as  $\phi_0 = hc/e$ ), formed when electrons confined to two dimensions are exposed to a strong magnetic field [8–10]. According to this theory, the interacting electrons at the Landau level (LL) filling factor  $\nu = n/(2pn \pm 1)$ ,  $n$  and  $p$  being integers, transform into weakly interacting composite fermions at an effective filling  $\nu^* = n$ ; the ground state corresponds to  $n$  filled CF Landau levels (CF-LLs) and it is natural to expect that the neutral excitations correspond to a particle-hole pair of composite fermions, called the CF exciton (Fig. 1a) [11,12]. At the minimum in its dispersion, the CF exciton is called the roton, borrowing the terminology from the  $^4\text{He}$  literature [2].

We will use the spherical geometry [13] below, which considers  $N$  electrons on the surface of a sphere in the presence of a radial magnetic field emanating from a magnetic monopole of strength  $Q$ , which corresponds to a total flux of  $2Q\phi_0$  through the surface of the sphere. The wave function for the CF ground state or the CF exciton at  $\nu = n/(2pn + 1)$ , denoted by  $\Psi$ , is constructed by analogy to the wave function of the corresponding elec-

tron states at  $\nu = n$ , denoted by  $\Phi$ :

$$\Psi = \mathcal{P}_{LLL} \Phi_1^{2p} \Phi \quad (1)$$

Here  $\Phi_1$  is the wavefunction of the fully occupied lowest Landau level with monopole strength equal to  $(N - 1)/2$ , given by  $\prod_{j < k} (u_j v_k - u_k v_j)$ , with  $u_j \equiv \cos(\theta_j/2) \exp(-i\phi_j/2)$  and  $v_j \equiv \sin(\theta_j/2) \exp(i\phi_j/2)$ .  $\mathcal{P}_{LLL}$  denotes projection of the wave function into the lowest Landau level (LLL). The monopole strengths for  $\Phi$  and  $\Psi$ ,  $q$  and  $Q$ , respectively, are related by  $Q = q + p(N - 1)$ . For the ground state and the single exciton, the wave functions  $\Phi$  are completely determined by symmetry (i.e., by fixing the total orbital angular momentum  $L$ , which is preserved in going from  $\Phi$  to  $\Psi$  according to the above rule), giving parameter-free wave functions  $\Psi$  for the ground and excited states of interacting electrons. These have been found to be extremely accurate in tests against exact diagonalization results available for small systems [8,14], establishing the essential validity of the CF exciton description of the neutral mode of the FQHE. However, these small system studies do not test the long wavelength limit, and there are indications that the single exciton might not be the lowest energy excitation in the long-wavelength limit. First, the agreement between the exact eigenenergy and the CF-exciton energy worsens somewhat at small  $k$ , indicating the possibility of new physics here. (The wave vector  $k$  is related to the orbital angular momentum  $L$  in the spherical geometry as  $k = L/R$ .) Secondly,  $\mathcal{P}_{LLL}$  projects away an increasingly bigger fraction of the single-exciton wave function as  $k \rightarrow 0$ , [11] eventually annihilating it completely. (This happens precisely at  $L = 1$  in the spherical geometry. [15]) Furthermore, in the thermodynamic limit, the energy of the single CF exciton in the  $k \rightarrow 0$  limit is slightly more than twice the energy of the CF roton, which raises the question of whether the two-roton excitation wins in the long wavelength limit. These observations have motivated us to look into the  $k \rightarrow 0$  limit in more detail.

We start by constructing a wave function  $\Psi$  for an excitation consisting of two CF excitons, for which we appeal to the analogy to the two-exciton state at  $\nu = n$ , which contains two particle-hole pairs, as shown in Fig. (1).

There are certain technical difficulties that one encounters in going from  $\Phi$  to  $\Psi$ . First, the final wave function is not automatically orthogonal to the *single* exciton wave function or the ground state wave function at the same  $L$ . In order to avoid the need for complicated Gram-Schmidt orthogonalization, we exploit the fortunate coincidence that there is no single exciton state at  $L = 1$  in the spherical geometry [15]. Therefore, we construct the two-roton wave function at  $L = 1$  and compare it with the single exciton at  $L = 2$ , both of which correspond to  $k \rightarrow 0$  in the thermodynamic limit. The second difficulty is that the wave function of the two-exciton is not unique at  $L = 1$ . A large number of combinations of two single excitons give a state at  $L = 1$ : one could combine either two single excitons with the same angular momenta or angular momenta differing by unity. We have discovered in our calculations that, in the former case, the LLL projection operator annihilates  $\Psi$ . Therefore, we construct  $\Phi_{q;L,M}^{TE}$ , the two-exciton state at  $q$  with quantum numbers  $L = 1$  and  $M = 0$ , from two single excitons at  $L_{SE}$  and  $L_{SE} + 1$  as shown in Fig. (1). The two-CF-exciton state at  $Q = q + p(N - 1)$ ,  $\Psi_{Q;L,M}^{TE}$ , is then constructed as:

$$\Psi_{Q;L,M}^{TE} = \mathcal{P}_{LLL} \Phi_1^{2p} \Phi_{q;L,M}^{TE} \quad (2)$$

One of the most challenging aspects of the desired computation is that the two-exciton CF state requires a very large number of Slater determinants; the number increases as  $N^3$ ,  $N$  being the number of electrons. For efficient Monte Carlo simulations we have devised a determinant-updating technique, generalizing the technique in Ref. [16]. The updating technique begins with the observation that the constituent Slater determinants of the two-exciton state differ from the ground state only in *two rows*. To elaborate on our updating method, first let  $[Y]_{\alpha,j}^{gs}$  denote an element of the matrix for the Slater determinant describing the ground state at  $q$ , i.e.  $\Phi_q^{gs}$ . Here  $\alpha$  collectively indicates orbital quantum numbers. Also, let  $\Phi_{m,m'+M_{SE}}^{m',m'-M_{SE}}(q,n)$  be the Hartree-Fock wavefunction obtained by promoting two composite fermions in the  $m$  and  $m'$  state of the topmost occupied CF-LL ( $(n-1)$ th CF-LL) to the  $m + M_{SE}$  and  $m' - M_{SE}$  state of the lowest unoccupied CF-LL ( $n$ -th CF-LL) which is depicted as the figure enclosed by square brackets in (b) of Fig. 1. Then,  $\Phi_{m,m'+M_{SE}}^{m',m'-M_{SE}}(q,n)$  is given by:

$$\begin{aligned} \Phi_q^{gs} & \left[ \left( \sum_j Y_{q,n,m+M_{SE}}(\Omega_j) [\overline{Y}]_{(q,n-1,m),j}^{gs} \right) \right. \\ & \times \left( \sum_j Y_{q,n,m'-M_{SE}}(\Omega_j) [\overline{Y}]_{(q,n-1,m'),j}^{gs} \right) \\ & \left. - \left( \sum_j Y_{q,n,m+M_{SE}}(\Omega_j) [\overline{Y}]_{(q,n-1,m'),j}^{gs} \right) \right] \end{aligned}$$

$$\times \left( \sum_j Y_{q,n,m'-M_{SE}}(\Omega_j) [\overline{Y}]_{(q,n-1,m),j}^{gs} \right) \quad (3)$$

where  $[\overline{Y}]^{gs}$  is the transpose of the inverse matrix of  $[Y]^{gs}$ . Eq. (3) reduces the number of operations by approximately a factor of  $N$ , compared to that of operations when the Slater determinants are computed separately. Then, using parallel computing techniques, such as message-passing interface (MPI), which reduces the (wall) computing time by another factor of 30 with as many as 64 processors, we are able to study systems with up to  $N = 30$  particles, which will be crucial in what follows.

The energies of the various two-exciton states (labeled by  $L_{SE}$ , or  $k_{SE} = L_{SE}/R$ ) are now evaluated for the pure Coulomb interaction by the Monte Carlo method, treating the LLL projection operator in the standard method [14]. The plot in Fig. 2 explicitly confirms that the lowest energy for each  $N$  is obtained by combining two *rotons*. In principle, the energy of the two-roton state could be further lowered by allowing it to mix with other two-exciton states, but this possibility will not be considered here. We have compared the energy of the two-roton state against exact diagonalization studies to ascertain the validity of the wave function. For  $N = 8$  and 10, energies per particle for the  $L = 1$  two-roton states in the composite fermion theory are  $-0.417440(46)$  and  $-0.416551(59)$  in units of  $e^2/\epsilon l_0$ , which are approximately 0.2% larger than the exact energies ( $-0.418324$  for  $N = 8$  and  $-0.417516$  for  $N = 10$ ). The CF energy gap at  $L = 1$  is approximately 5% higher than the exact value.

Fig. 3 shows the evolution of the energies of the single exciton and the two-roton bound state as a function of  $N$ . This plot demonstrates the principal result of the work, namely that the lowest energy excitation in the long wavelength limit is the two-roton state. We note here that in the long wavelength limit, the single CF exciton is identical to the SMA mode [11], consistent with the fact in Fig. 3 that the energy of the single exciton approaches  $0.15 e^2/\epsilon l_0$  in the thermodynamic limit, which is also the  $k = 0$  energy of the SMA mode [2]. The two-roton state has 10% lower energy.

We next come to the relevance of this work to Raman scattering experiment. Our theoretical understanding of the scattering cross section of the FQHE gap modes observed in Raman scattering is rather unsatisfactory, even ignoring the complications introduced by the resonant nature of Raman scattering [17,7]. However, as noted in the early literature [3], there is reason to expect that the two-roton mode might couple more strongly to light in Raman scattering than the single exciton mode: the scattering cross section for the single exciton vanishes rapidly with the wave vector as a result of Kohn's theorem, but there is no reason for it to vanish for the two-roton mode. Also note that while the two-exciton states form a contin-

uum, the two-roton states provide a peak in the density of states at the lower edge of the continuum.

In a detailed study, Scarola *et al.* [12] have found that, after incorporating the finite thickness effect, the energy of the single CF-roton is in excellent agreement with experiment, but the energy of the mode observed in the long wave length limit is approximately 30% below the theoretical energy of the single exciton. In light of the above discussion, it is natural to suggest that a part of this discrepancy might originate from a misassignment of the nature of the long wavelength mode. In order to make contact with experiment at a quantitative level, we have considered a square quantum well (SQW) of width 33 nm, as appropriate for the experiment of Kang *et al.* [18] The transverse wave function has been calculated in a self-consistent local density approximation, as a function of the two-dimensional electron density, following which the integration over the transverse coordinate has been performed explicitly to obtain an effective two-dimensional interaction between electrons [19,20]. This, in turn, is used to compute the energy of the two-roton bound state. The thermodynamic limit is obtained at each density. The excitation energies are further reduced due to Landau level mixing, which was estimated by Scarola *et al.* as a function of the density for the single roton at  $\nu = 1/3$ , following earlier work [21]. Assuming that the percent reduction of the two-roton energy is approximately the same (approximately 5% for typical densities), we have obtained a realistic estimate for the energy of the two-roton mode, plotted (dashed line) in Fig. 4 along with the experimentally determined energies [18] of the long-wavelength mode (stars). The agreement is on the level of 20% or better, which we consider satisfactory in view of various approximations and the neglect of disorder.

Our calculations also show a level crossing between the two-roton and the single exciton modes at approximately  $\rho = 3.0 \times 10^{11} \text{ cm}^{-2}$  for the SQW sample of width 33nm. If only the two-roton mode is observable in Raman scattering, this would imply that the Raman peak ought to disappear at sufficiently large densities. The actual density at which the level crossing is predicted may be a quite sensitive function of the various approximations of the theory, however.

In summary, we have proved that at  $\nu = 1/3$  the lowest energy excitation in the long wavelength limit is not a single exciton but rather a two-roton mode. The results of Ref. [12] show that much of this physics is to be expected at other filling factors as well, since there also the  $k \rightarrow 0$  limit of the single exciton energy is larger than twice the single roton energy. Calculations are in progress to investigate this issue further. This work was supported in part by the National Science Foundation under grant no. DMR-9986806. We are grateful to Vito Scarola for numerous helpful discussions and the Numerically Intensive Computing Group led by V. Agarwala, J. Holmes, and J. Nucciarone, at the Penn State Uni-

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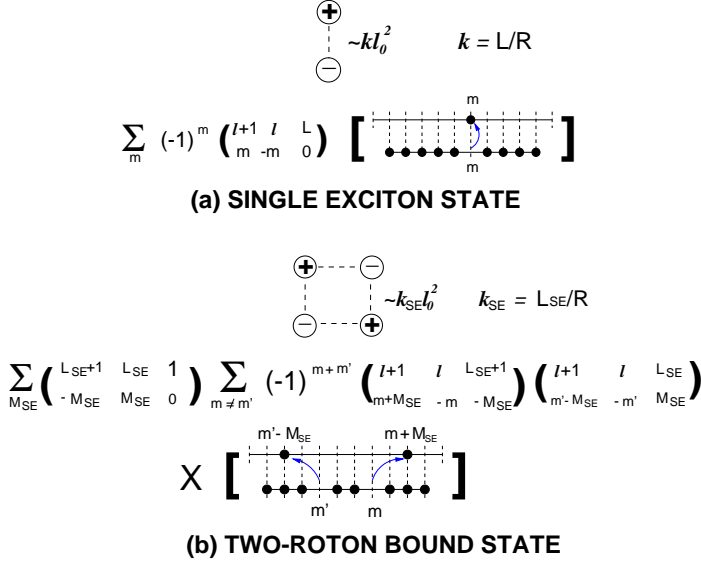


FIG. 1. Schematic diagrams for (a) the single exciton state and (b) the two-exciton state, with well defined  $L$  and  $M$  quantum numbers. (We have chosen  $M = 0$  with no loss of generality, since the energy is independent of  $M$ .) The figure in square brackets shows schematically the Hartree-Fock Slater determinant obtained by promoting one or two electrons from the topmost occupied Landau level to lowest unoccupied Landau level in single particle states indicated. At filling factor  $n$ , the topmost occupied (lowest unoccupied) LL corresponds to the angular momentum  $l = q + n - 1$  ( $l = q + n$ ) shell in the spherical geometry; other Landau level shells are not shown for simplicity. The Wigner 3-j symbols are used in order to make a definite angular-momentum eigenstate. The relative signs of the various terms in the sum follow from the antisymmetry requirement.

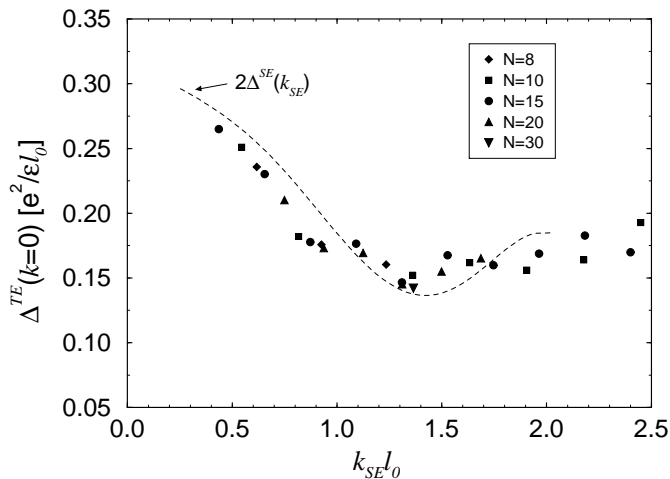


FIG. 2. The energies of various two-exciton states as a function of the wave vector of two constituent single excitons, which is denoted by  $k_{SE}$ . Here the interaction between electrons is taken as the Coulomb interaction. Comparison with twice the single exciton dispersion curve (dashed line) shows that the lowest-energy two-exciton state is obtained by combining two *rotons*.

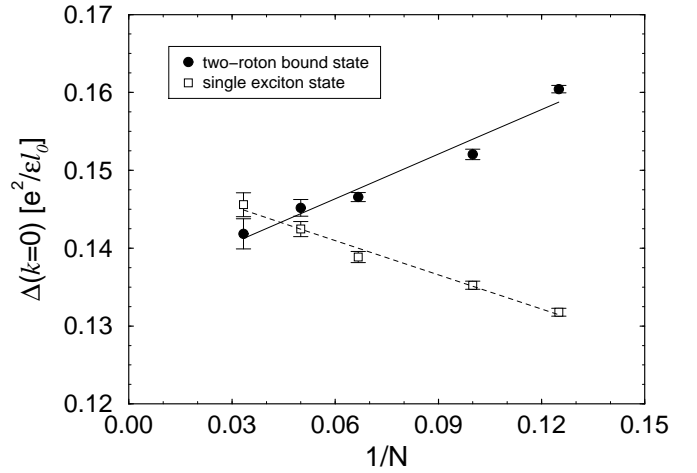


FIG. 3. The Coulomb energies as a function of  $1/N$  for the single exciton and the two-roton bound state in the long wavelength limit.

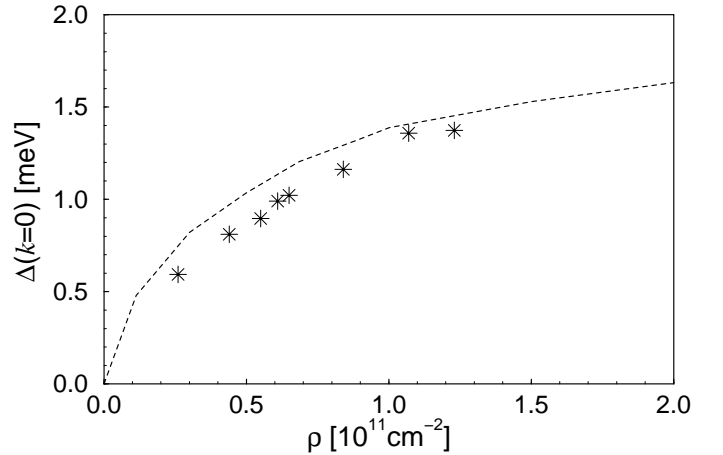


FIG. 4. Comparison between the experimental data (stars) from Kang *et al.* [18] and the theoretical estimation of two-roton bound state energy (dashed line). Theoretical estimates are obtained by considering Landau level mixing as well as finite thickness effects.